

10/717,958

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NEWS	2		"Ask CAS" for self-help around the clock
NEWS	3	SEP 01	New pricing for the Save Answers for SciFinder Wizard within STN Express with Discover!
NEWS	4	OCT 28	KOREAPAT now available on STN
NEWS	5	NOV 30	PHAR reloaded with additional data
NEWS	6	DEC 01	LISA now available on STN
NEWS	7	DEC 09	12 databases to be removed from STN on December 31, 2004
NEWS	8	DEC 15	MEDLINE update schedule for December 2004
NEWS	9	DEC 17	ELCOM reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	10	DEC 17	COMPUAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	11	DEC 17	SOLIDSTATE reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	12	DEC 17	CERAB reloaded; updating to resume; current-awareness alerts (SDIs) affected
NEWS	13	DEC 17	THREE NEW FIELDS ADDED TO IFIPAT/IFIUDB/IFICDB
NEWS	14	DEC 30	EPFULL: New patent full text database to be available on STN
NEWS	15	DEC 30	CAPLUS - PATENT COVERAGE EXPANDED
NEWS	16	JAN 03	No connect-hour charges in EPFULL during January and February 2005
NEWS	17	FEB 25	CA/CAPLUS - Russian Agency for Patents and Trademarks (ROSPATENT) added to list of core patent offices covered
NEWS	18	FEB 10	STN Patent Forums to be held in March 2005
NEWS	19	FEB 16	STN User Update to be held in conjunction with the 229th ACS National Meeting on March 13, 2005
NEWS	20	FEB 28	PATDPAFULL - New display fields provide for legal status data from INPADOC
NEWS	21	FEB 28	BABS - Current-awareness alerts (SDIs) available
NEWS	22	FEB 28	MEDLINE/LMEDLINE reloaded
NEWS	23	MAR 02	GBFULL: New full-text patent database on STN
NEWS	24	MAR 03	REGISTRY/ZREGISTRY - Sequence annotations enhanced
NEWS	25	MAR 03	MEDLINE file segment of TOXCENTER reloaded
NEWS EXPRESS			JANUARY 10 CURRENT WINDOWS VERSION IS V7.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 10 JANUARY 2005
NEWS HOURS			STN Operating Hours Plus Help Desk Availability
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FILE 'HOME' ENTERED AT 16:22:25 ON 15 MAR 2005

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 16:22:39 ON 15 MAR 2005

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STRUCTURE FILE UPDATES: 14 MAR 2005 HIGHEST RN 845540-96-7

DICTIONARY FILE UPDATES: 14 MAR 2005 HIGHEST RN 845540-96-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 18, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

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<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

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L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 16:22:57 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 350 TO ITERATE

100.0% PROCESSED 350 ITERATIONS

8 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*

BATCH \*\*COMPLETE\*\*

PROJECTED ITERATIONS: 5878 TO 8122

PROJECTED ANSWERS: 8 TO 329

L2 8 SEA SSS SAM L1

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=> s l1 ful

FULL SEARCH INITIATED 16:23:05 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 7356 TO ITERATE

100.0% PROCESSED 7356 ITERATIONS  
SEARCH TIME: 00.00.01

124 ANSWERS

L3 124 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
161.33	161.54

FULL ESTIMATED COST

FILE 'CAPLUS' ENTERED AT 16:23:13 ON 15 MAR 2005  
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FILE COVERS 1907 - 15 Mar 2005 VOL 142 ISS 12  
FILE LAST UPDATED: 14 Mar 2005 (20050314/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l3

L4 19 L3

=> s l4 and (process or making or make or made or prepar? or syntheses?)

2060830 PROCESS  
1374299 PROCESSES  
3065131 PROCESS  
(PROCESS OR PROCESSES)  
244396 MAKING  
30 MAKINGS  
244420 MAKING  
(MAKING OR MAKINGS)  
205723 MAKE  
158981 MAKES  
354430 MAKE  
(MAKE OR MAKES)  
1138680 MADE  
23 MADES  
1138700 MADE  
(MADE OR MADES)  
1534101 PREPAR?  
115055 PREP

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2025 PREPS  
116881 PREP  
    (PREP OR PREPS)  
1918786 PREPD  
    21 PREPDS  
1918801 PREPD  
    (PREPD OR PREPDS)  
106004 PREPG  
    12 PREPGS  
106015 PREPG  
    (PREPG OR PREPGS)  
2557303 PREPN  
198667 PREPNS  
2707792 PREPN  
    (PREPN OR PREPNS)  
4488110 PREPAR?  
    (PREPAR? OR PREP OR PREPD OR PREPG OR PREPN)  
1433499 SYNTHES?  
L5 9 L4 AND (PROCESS OR MAKING OR MAKE OR MADE OR PREPAR? OR SYNTHES?  
    )

=> d l5 ibib hitstr abs 1-9

L5 ANSWER 1 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2004:567636 CAPLUS  
DOCUMENT NUMBER: 141:290174  
TITLE: Structural Bioinformatics and QSAR Analysis Applied to  
the Acetylcholinesterase and Bispyridinium Aldoximes  
AUTHOR(S): Mager, Peter; Weber, Anje  
CORPORATE SOURCE: Research Group of Pharmacochemistry, Institute of  
Pharmacology and Toxicology, Univ. Leipzig, Saxony,  
Germany  
SOURCE: Drug Design and Discovery (2003), 18(4), 127-150  
CODEN: DDDIEV; ISSN: 1055-9612  
PUBLISHER: Taylor & Francis, Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
IT 84871-04-5  
RL: BSU (Biological study, unclassified); PRP (Properties); BIOL  
(Biological study)  
(QSAR anal. applied to acetylcholinesterase and bispyridinium aldoximes  
for qual. structural requirements for reactivating activity against  
organophosphorus agents)  
RN 84871-04-5 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[[[4-[(hydroxyimino)methyl]pyridinio]methoxy]methyl]- (9CI) (CA INDEX NAME)

/ Structure 1 in file .gra /

AB The methods of bioinformatics, mol. modeling, and quant.  
structure-activity relationships (QSARs) using regression and artificial  
neural network (ANN) analyses were applied to develop safer aldoxime  
antidotes against poisoning by organophosphorus (OP) agents with high,  
mean, and low aging rates. We start here from a mol. modeling of the  
mouse AChE at an atomistic level. Aim is to predict qual. the structural  
requirements of an aldoxime that shows an unique reactivating activity  
against the three classes of OPs. An antidotal action should occur by a  
three-site mechanism: the aldoxime groups of the first pyridinium ring  
should point towards the catalytic site, and the second pyridinium ring

and its substituents should be anchored at the peripheral and anionic subsites. Based on this model, it is predicted that a suitable substituent is based on an arginine-like moiety. Then, an ANN-based QSAR anal. using a training set of aldoximes with known structure and activities was applied. Its input layer consisted of seven nodes: the group-membership descriptors that parameterize the type of the OP, the logarithms of the distribution coeffs. at pH 7.4 and their squared term, the LUMO energies, the scaled molar refractions of the substituents, and their squared term. It was shown that the qual. prediction made by mol. modeling can be quantified by an ANN prediction.

REFERENCE COUNT: 70 THERE ARE 70 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:258121 CAPLUS

DOCUMENT NUMBER: 140:425258

TITLE: **Synthesis** and Aqueous Ozonation of Some Pyridinium Salts with Alkoxymethyl and Alkylthiomethyl Hydrophobic Groups

AUTHOR(S): Pernak, Juliusz; Branicka, Monika

CORPORATE SOURCE: Institute of Chemical Technology and Engineering, Poznan University of Technology, Poznan, 60-965, Pol.

SOURCE: Industrial & Engineering Chemistry Research (2004), 43(9), 1966-1974

CODEN: IECRED; ISSN: 0888-5885

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 571205-42-0P 571205-43-1P 571205-44-2P

571205-45-3P 571205-46-4P 571205-47-5P

571205-48-6P 571205-49-7P 571205-50-0P

RL: BUU (Biological use, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation and aqueous ozonation of some pyridinium salts with alkoxymethyl and alkylthiomethyl hydrophobic groups)

RN 571205-42-0 CAPLUS

CN Pyridinium, 3-(dimethylamino)-1-[(heptyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 2 in file .gra /

RN 571205-43-1 CAPLUS

CN Pyridinium, 3-(dimethylamino)-1-[(octyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 3 in file .gra /

RN 571205-44-2 CAPLUS

CN Pyridinium, 3-(dimethylamino)-1-[(nonyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 4 in file .gra /

RN 571205-45-3 CAPLUS

CN Pyridinium, 1-[(decyloxy)methyl]-3-(dimethylamino)-, chloride (9CI) (CA INDEX NAME)

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/ Structure 5 in file .gra /

RN 571205-46-4 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[(undecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 6 in file .gra /

RN 571205-47-5 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[(dodecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 7 in file .gra /

RN 571205-48-6 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[(tetradecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 8 in file .gra /

RN 571205-49-7 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[(hexadecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 9 in file .gra /

RN 571205-50-0 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[(octadecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 10 in file .gra /

AB The reaction of ozone with a number of pyridinium salts containing 1-alkoxymethyl and 1-alkylthiomethyl substituents was determined at a total substrate concentration of 2 g/L. Ozonation of pyridinium salts was strongly dependent on the kinds and positions of the substituents in the pyridine ring. The most favorable were the third position and the substituents including hydroxyl or dimethylamino groups. In an aqueous solution, 1-(alkoxymethyl)-3-hydroxypyridinium, 1-(alkylthiomethyl)-3-hydroxypyridinium, and 1-(alkoxymethyl)-3-(dimethylamino)pyridinium salts reacted with ozone. The reaction was fast, and pyridinium salts were quant. removed. 1-(Alkoxymethyl)- and 1-(alkylthiomethyl)pyridinium chlorides were obtained by the Menschutkin reaction. In general, the procedure was simple and the reaction was productive and short. During the course of this study, we synthesized a new generation of cationic surfactants that were extremely reactive with ozone in an aqueous solution

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 2003:346161 CAPLUS  
DOCUMENT NUMBER: 139:149500

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TITLE: The properties of 1-alkoxymethyl-3-hydroxypyridinium  
and 1-alkoxymethyl-3-dimethylaminopyridinium chlorides  
AUTHOR(S): Pernak, Juliusz; Branicka, Monika  
CORPORATE SOURCE: Department of Chemical Technology, Poznan University  
of Technology, Poznan, 60-965, Pol.  
SOURCE: Journal of Surfactants and Detergents (2003), 6(2),  
119-123  
CODEN: JSDEFL; ISSN: 1097-3958  
PUBLISHER: AOCS Press  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 139:149500  
IT 571205-38-4P 571205-39-5P 571205-40-8P  
571205-41-9P 571205-42-0P 571205-43-1P  
571205-44-2P 571205-45-3P 571205-46-4P  
571205-47-5P 571205-48-6P 571205-49-7P  
571205-50-0P  
RL: BSU (Biological study, unclassified); SPN (Synthetic preparation);  
BIOL (Biological study); PREP (Preparation)  
(preps. and antimicrobial activities of 1-alkoxymethyl-3-  
substituted pyridinium chlorides)  
RN 571205-38-4 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-(propoxymethyl)-, chloride (9CI) (CA  
INDEX NAME)

/ Structure 11 in file .gra /

RN 571205-39-5 CAPLUS  
CN Pyridinium, 1-(butoxymethyl)-3-(dimethylamino)-, chloride (9CI) (CA INDEX  
NAME)

/ Structure 12 in file .gra /

RN 571205-40-8 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[(pentyloxy)methyl]-, chloride (9CI) (CA  
INDEX NAME)

/ Structure 13 in file .gra /

RN 571205-41-9 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[(hexyloxy)methyl]-, chloride (9CI) (CA  
INDEX NAME)

/ Structure 14 in file .gra /

RN 571205-42-0 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[(heptyloxy)methyl]-, chloride (9CI) (CA  
INDEX NAME)

/ Structure 15 in file .gra /

RN 571205-43-1 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[(octyloxy)methyl]-, chloride (9CI) (CA  
INDEX NAME)

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/ Structure 16 in file .gra /

RN 571205-44-2 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[(nonyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 17 in file .gra /

RN 571205-45-3 CAPLUS  
CN Pyridinium, 1-[(decyloxy)methyl]-3-(dimethylamino)-, chloride (9CI) (CA INDEX NAME)

/ Structure 18 in file .gra /

RN 571205-46-4 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[(undecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 19 in file .gra /

RN 571205-47-5 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[(dodecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 20 in file .gra /

RN 571205-48-6 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[(tetradecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 21 in file .gra /

RN 571205-49-7 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[(hexadecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 22 in file .gra /

RN 571205-50-0 CAPLUS  
CN Pyridinium, 3-(dimethylamino)-1-[(octadecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 23 in file .gra /

AB Several 1-alkoxymethyl-3-substituted-pyridinium chlorides with alkoxy chains including from 3 to 18 carbon atoms were **prepared** by the reaction of 3-substituted-pyridine with chloromethyl alkyl ethers. The **prepared** chlorides were examined for their antielectrostatic effects and their antimicrobial activities. 1-Dodecyloxymethyl-3-dimethylaminopyridinium chloride (23) exhibited strong antimicrobial activity and a wide antimicrobial spectrum, similar to the activity of benzalkonium chloride. 1-Alkoxymethyl-3-hydroxypyridinium chlorides



possess antielectrostatic properties, but are lacking antimicrobial activity. The antielectrostatic effect and antimicrobial activities are strongly dependent on the kind of substituent at the 3-position in the pyridine ring and are greatly affected by an alkoxy chain. Dimethylamino group in position three must be present for a high antielectrostatic and antimicrobial activity of the agent.

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:325907 CAPLUS

DOCUMENT NUMBER: 137:201262

TITLE: **Synthesis** and antimicrobial activities of new pyridinium and benzimidazolium chlorides

AUTHOR(S): Pernak, Juliusz; Rogoza, Jarostaw; Mirska, Ilona

CORPORATE SOURCE: Poznan University of Technology, Poznan, 60-965, Pol.

SOURCE: European Journal of Medicinal Chemistry (2001), 36(4), 313-320

CODEN: EJMCA5; ISSN: 0223-5234

PUBLISHER: Editions Scientifiques et Medicales Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 137:201262

IT 404965-60-2P 452281-20-8P 452281-21-9P

452281-22-0P

RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)

(**synthesis** and antibacterial and antifungal activities of new pyridinium and benzimidazolium chlorides)

RN 404965-60-2 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(undecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 24 in file .gra /

RN 452281-20-8 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(nonyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 25 in file .gra /

RN 452281-21-9 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(decyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 26 in file .gra /

RN 452281-22-0 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 27 in file .gra /

IT 404965-58-8P 404965-59-9P 404965-71-5P

404965-72-6P 404965-84-0P 404965-85-1P

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404965-86-2P 404965-87-3P 404965-88-4P  
404965-89-5P 404965-90-8P 404965-91-9P  
404965-92-0P 404965-93-1P 452281-16-2P  
452281-17-3P 452281-18-4P 452281-19-5P  
452281-23-1P 452281-24-2P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL  
(Biological study); PREP (Preparation)

(**synthesis** and antibacterial and antifungal activities of new  
pyridinium and benzimidazolium chlorides)

RN 404965-58-8 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-(propoxymethyl)-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 28 in file .gra /

RN 404965-59-9 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 29 in file .gra /

RN 404965-71-5 CAPLUS

CN Pyridinium, 3,3'-(methylenediimino)bis[1-[(nonyloxy)methyl]-, dichloride  
(9CI) (CA INDEX NAME)

/ Structure 30 in file .gra /

RN 404965-72-6 CAPLUS

CN Pyridinium, 3,3'-(methylenediimino)bis[1-(undecyloxy)methyl]-, dichloride  
(9CI) (CA INDEX NAME)

/ Structure 31 in file .gra /

RN 404965-84-0 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 32 in file .gra /

RN 404965-85-1 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(butoxymethyl)-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 33 in file .gra /

RN 404965-86-2 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(pentyloxy)methyl]-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 34 in file .gra /

RN 404965-87-3 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(hexyloxy)methyl]-,

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chloride (9CI) (CA INDEX NAME)

/ Structure 35 in file .gra /

RN 404965-88-4 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(heptyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 36 in file .gra /

RN 404965-89-5 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 37 in file .gra /

RN 404965-90-8 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(nonyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 38 in file .gra /

RN 404965-91-9 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(decyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 39 in file .gra /

RN 404965-92-0 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(undecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 40 in file .gra /

RN 404965-93-1 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 41 in file .gra /

RN 452281-16-2 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-(butoxymethyl)-, chloride (9CI) (CA INDEX NAME)

/ Structure 42 in file .gra /

RN 452281-17-3 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(pentyloxy)methyl]-, chloride (9CI) (CA INDEX NAME)

/ Structure 43 in file .gra /

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RN 452281-18-4 CAPLUS  
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(hexyloxy)methyl]-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 44 in file .gra /

RN 452281-19-5 CAPLUS  
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(heptyloxy)methyl]-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 45 in file .gra /

RN 452281-23-1 CAPLUS  
CN Pyridinium, 3,3'-(methylenediimino)bis[1-[(decyloxy)methyl]-, dichloride  
(9CI) (CA INDEX NAME)

/ Structure 46 in file .gra /

RN 452281-24-2 CAPLUS  
CN Pyridinium, 3,3'-(methylenediimino)bis[1-[(dodecyloxy)methyl]-, dichloride  
(9CI) (CA INDEX NAME)

/ Structure 47 in file .gra /

GI

/ Structure 48 in file .gra /

AB Novel pyridinium, e.g I, and benzimidazolium, e.g. II, chlorides were obtained in high yield. The antimicrobial activities of three homologous series of pyridinium and benzimidazolium chlorides against cocci, rods, fungi and bacillus were measured. The antimicrobial activities of N,N'-bis[3-(1-alkoxymethyl)pyridinium chloride]methylenediamines, 1-undecyloxymethyl-3-(1-benzimidazolmethylamino)pyridinium, 1-undecyloxymethyl- and 1-dodecyloxymethyl-3-[1(benzotriazol-1-yl)methylamino]pyridinium chlorides exhibited strong activity and wide antibacterial spectra similar to the activity of benzalkonium chloride.

REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:773384 CAPLUS

DOCUMENT NUMBER: 136:263127

TITLE: **Synthesis** of 3-substituted pyridinium salts

AUTHOR(S): Pernak, Juliusz; Rogoza, Jaroslaw

CORPORATE SOURCE: Inst. Chem. Technol. Eng., Poznan Univ. Technol.,  
Poznan, 60-965, Pol.

SOURCE: ARKIVOC [online computer file] (2000), 1(6), 889-904

CODEN: AKVCFI

URL: <http://www.arkat.org/arkat/journal/Issue6/ms06-0084.pdf>

10/717,958

PUBLISHER: ARKAT Foundation  
DOCUMENT TYPE: Journal; (online computer file)  
LANGUAGE: English  
IT 404965-58-8P 404965-59-9P 404965-60-2P  
404965-61-3P 404965-63-5P 404965-64-6P  
404965-65-7P 404965-66-8P 404965-67-9P  
404965-68-0P 404965-70-4P 404966-06-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of 3-substituted pyridinium salts)  
RN 404965-58-8 CAPLUS  
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-(propoxymethyl)-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 49 in file .gra /

RN 404965-59-9 CAPLUS  
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 50 in file .gra /

RN 404965-60-2 CAPLUS  
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(undecyloxy)methyl]-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 51 in file .gra /

RN 404965-61-3 CAPLUS  
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-(propoxymethyl)-,  
bromide (9CI) (CA INDEX NAME)

/ Structure 52 in file .gra /

RN 404965-63-5 CAPLUS  
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,  
nitrate (9CI) (CA INDEX NAME)

CM 1

CRN 404965-62-4  
CMF C22 H31 N4 O

/ Structure 53 in file .gra /

CM 2

CRN 14797-55-8  
CMF N O3

/ Structure 54 in file .gra /

RN 404965-64-6 CAPLUS

10/717,958

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,  
iodide (9CI) (CA INDEX NAME)

/ Structure 55 in file .gra /

RN 404965-65-7 CAPLUS  
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,  
tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 404965-62-4  
CMF C22 H31 N4 O

/ Structure 56 in file .gra /

CM 2

CRN 14874-70-5  
CMF B F4  
CCI CCS

/ Structure 57 in file .gra /

RN 404965-66-8 CAPLUS  
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,  
hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 404965-62-4  
CMF C22 H31 N4 O

/ Structure 58 in file .gra /

CM 2

CRN 16919-18-9  
CMF F6 P  
CCI CCS

/ Structure 59 in file .gra /

RN 404965-67-9 CAPLUS  
CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,  
perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 404965-62-4  
CMF C22 H31 N4 O

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/ Structure 60 in file .gra /

CM 2

CRN 14797-73-0

CMF Cl O4

/ Structure 61 in file .gra /

RN 404965-68-0 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-,  
iodide (9CI) (CA INDEX NAME)

/ Structure 62 in file .gra /

RN 404965-70-4 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-,  
hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 404965-69-1

CMF C26 H39 N4 O

/ Structure 63 in file .gra /

CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS

/ Structure 64 in file .gra /

RN 404966-06-9 CAPLUS

CN Pyridinium, 3-[(1H-benzimidazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-,  
perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 404965-69-1

CMF C26 H39 N4 O

/ Structure 65 in file .gra /

CM 2

CRN 14797-73-0

CMF Cl O4

/ Structure 66 in file .gra /

10/717,958

IT 404965-71-5P 404965-72-6P 404965-74-8P  
404965-75-9P 404965-76-0P 404965-77-1P  
404965-79-3P 404965-80-6P 404965-81-7P  
404965-84-0P 404965-85-1P 404965-86-2P  
404965-87-3P 404965-88-4P 404965-89-5P  
404965-90-8P 404965-91-9P 404965-92-0P  
404965-93-1P 404965-94-2P 404965-96-4P  
404965-98-6P 404965-99-7P 404966-00-3P  
404966-01-4P 404966-02-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of 3-substituted pyridinium salts)

RN 404965-71-5 CAPLUS

CN Pyridinium, 3,3'-(methylenediimino)bis[1-[(nonyloxy)methyl]-, dichloride  
(9CI) (CA INDEX NAME)

/ Structure 67 in file .gra /

RN 404965-72-6 CAPLUS

CN Pyridinium, 3,3'-(methylenediimino)bis[1-(undecyloxy)methyl]-, dichloride  
(9CI) (CA INDEX NAME)

/ Structure 68 in file .gra /

RN 404965-74-8 CAPLUS

CN Pyridinium, 3,3'-(methylenediimino)bis[1-[(octyloxy)methyl]-,  
diperchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 404965-73-7

CMF C29 H50 N4 O2

/ Structure 69 in file .gra /

CM 2

CRN 14797-73-0

CMF Cl O4

/ Structure 70 in file .gra /

RN 404965-75-9 CAPLUS

CN Pyridinium, 3,3'-(methylenediimino)bis[1-[(octyloxy)methyl]-, dibromate  
(9CI) (CA INDEX NAME)

CM 1

CRN 404965-73-7

CMF C29 H50 N4 O2

/ Structure 71 in file .gra /



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CM 2

CRN 15541-45-4

CMF Br O3

/ Structure 72 in file .gra /

RN 404965-76-0 CAPLUS

CN Pyridinium, 3,3'-(methylenediimino)bis[1-(octyloxy)methyl]-, diiodide  
(9CI) (CA INDEX NAME)

/ Structure 73 in file .gra /

RN 404965-77-1 CAPLUS

CN Pyridinium, 3,3'-(methylenediimino)bis[1-(octyloxy)methyl]-, dibromide  
(9CI) (CA INDEX NAME)

/ Structure 74 in file .gra /

RN 404965-79-3 CAPLUS

CN Pyridinium, 3,3'-(methylenediimino)bis[1-[(dodecyloxy)methyl]-,  
bis[hexafluorophosphate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 404965-78-2

CMF C37 H66 N4 O2

/ Structure 75 in file .gra /

CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS

/ Structure 76 in file .gra /

RN 404965-80-6 CAPLUS

CN Pyridinium, 3,3'-(methylenediimino)bis[1-[(dodecyloxy)methyl]-,  
bis[(OC-6-11)-hexafluoroantimonate(1-)] (9CI) (CA INDEX NAME)

CM 1

CRN 404965-78-2

CMF C37 H66 N4 O2

/ Structure 77 in file .gra /

CM 2

CRN 17111-95-4

10/717,958

CMF F6 Sb  
CCI CCS

/ Structure 78 in file .gra /

RN 404965-81-7 CAPLUS  
CN Pyridinium, 3,3'-(methylenediimino)bis[1-(dodecyloxy)methyl]-, diiodide  
(9CI) (CA INDEX NAME)

/ Structure 79 in file .gra /

RN 404965-84-0 CAPLUS  
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 80 in file .gra /

RN 404965-85-1 CAPLUS  
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(butoxymethyl)-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 81 in file .gra /

RN 404965-86-2 CAPLUS  
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(pentyloxy)methyl]-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 82 in file .gra /

RN 404965-87-3 CAPLUS  
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(hexyloxy)methyl]-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 83 in file .gra /

RN 404965-88-4 CAPLUS  
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(heptyloxy)methyl]-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 84 in file .gra /

RN 404965-89-5 CAPLUS  
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(octyloxy)methyl]-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 85 in file .gra /

RN 404965-90-8 CAPLUS  
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(nonyloxy)methyl]-,  
chloride (9CI) (CA INDEX NAME)

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/ Structure 86 in file .gra /

RN 404965-91-9 CAPLUS  
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(decyloxy)methyl]-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 87 in file .gra /

RN 404965-92-0 CAPLUS  
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(undecyloxy)methyl]-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 88 in file .gra /

RN 404965-93-1 CAPLUS  
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-[(dodecyloxy)methyl]-,  
chloride (9CI) (CA INDEX NAME)

/ Structure 89 in file .gra /

RN 404965-94-2 CAPLUS  
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-,  
iodide (9CI) (CA INDEX NAME)

/ Structure 90 in file .gra /

RN 404965-96-4 CAPLUS  
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-,  
(OC-6-11)-hexafluoroantimonate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 404965-95-3  
CMF C16 H20 N5 O

/ Structure 91 in file .gra /

CM 2

CRN 17111-95-4  
CMF F6 Sb  
CCI CCS

/ Structure 92 in file .gra /

RN 404965-98-6 CAPLUS  
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(butoxymethyl)-,  
perchlorate (9CI) (CA INDEX NAME)

CM 1

CRN 404965-97-5  
CMF C17 H22 N5 O

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/ Structure 93 in file .gra /

CM 2

CRN 14797-73-0

CMF Cl O4

/ Structure 94 in file .gra /

RN 404965-99-7 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(butoxymethyl)-, nitrate (9CI) (CA INDEX NAME)

CM 1

CRN 404965-97-5

CMF C17 H22 N5 O

/ Structure 95 in file .gra /

CM 2

CRN 14797-55-8

CMF N O3

/ Structure 96 in file .gra /

RN 404966-00-3 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 404965-95-3

CMF C16 H20 N5 O

/ Structure 97 in file .gra /

CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS

/ Structure 98 in file .gra /

RN 404966-01-4 CAPLUS

CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(propoxymethyl)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

10/717,958

CM 1

CRN 404965-95-3  
CMF C16 H20 N5 O

/ Structure 99 in file .gra /

CM 2

CRN 14874-70-5  
CMF B F4  
CCI CCS

/ Structure 100 in file .gra /

RN 404966-02-5 CAPLUS  
CN Pyridinium, 3-[(1H-benzotriazol-1-ylmethyl)amino]-1-(butoxymethyl)-,  
iodide (9CI) (CA INDEX NAME)

/ Structure 101 in file .gra /

AB A novel class of 3-substituted pyridinium salts have been  
**synthesized** in high yield by a convenient two-step procedure. A  
new synthetic pathway to 1-substituted benzimidazolium salts has been  
developed and the effects of the anionic component of the salts have been  
studied.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1989:614902 CAPLUS  
DOCUMENT NUMBER: 111:214902  
TITLE:  $\alpha,\omega$ -Di(phosphonomethyl) and  
 $\alpha,\omega$ -di(methylphosphinomethyl)  
L- $\alpha,\omega$ -diamino acids  
AUTHOR(S): Nachev, I.  
CORPORATE SOURCE: Res. Cent. "Konstrukcionni Polimeri", Sofia, 1528,  
Bulg.  
SOURCE: Izvestiya po Khimiya (1988), 21(4), 477-83  
CODEN: IZKHDX; ISSN: 0324-0401  
DOCUMENT TYPE: Journal  
LANGUAGE: Bulgarian  
OTHER SOURCE(S): CASREACT 111:214902  
IT 123529-71-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(**preparation** and reactions with Et phosphite or methylphosphonite)  
RN 123529-71-5 CAPLUS  
CN Acetamide, N-[(acetyloxy)methyl]-N-[1-[(acetyloxy)methyl]-2-oxo-3-  
piperidinyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ Structure 102 in file .gra /

GI

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/ Structure 103 in file .gra /

AB Treatment of the lactams of L-2,4-diaminobutanoic acid, L-ornithine, or L-lysine with HCHO in the presence 1,10-phenanthroline Co complex, followed by (CF<sub>3</sub>CO)<sub>2</sub>O in AcOH, afforded acetoxymethylated derivs. I (n = 1, 2, 3; R = AcOH). Condensation of the latter with P(OEt)<sub>3</sub> or MeP(OEt)<sub>2</sub> gave phosphorus derivs. I [R = R<sub>1</sub>P(O)OEt, R<sub>1</sub> = OEt, Me]. Hydrolysis of the P ester groups with phosphodiesterase I and alkaline hydrolysis of the lactam ring and the acetyl group afforded title amino acids  
HOPR1(O)CH<sub>2</sub>NHCH(CO<sub>2</sub>)<sub>n</sub>+1NHCH<sub>2</sub>PR1(O)OH.

L5 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1978:542494 CAPLUS  
DOCUMENT NUMBER: 89:142494  
TITLE: Aging of soman-inhibited acetylcholinesterase: inhibitors and accelerators  
AUTHOR(S): Schoene, K.  
CORPORATE SOURCE: Inst. Aerobiol., Fraunhofer-Ges., Schmallenberg-Grafschaft, Fed. Rep. Ger.  
SOURCE: Biochimica et Biophysica Acta (1978), 525(2), 468-71  
CODEN: BBACAQ; ISSN: 0006-3002  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
IT 61360-43-8 61368-95-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, with soman-inhibited acetylcholinesterase, aging in relation to)  
RN 61360-43-8 CAPLUS  
CN Pyridinium, 1,1'-[oxybis(methylene)]bis[3-[(aminocarbonyl)amino]-, dichloride (9CI) (CA INDEX NAME)

/ Structure 104 in file .gra /

RN 61368-95-4 CAPLUS  
CN Pyridinium, 1,1'-[oxybis(methylene)]bis[3-(acetylamino)-, dichloride (9CI) (CA INDEX NAME)

/ Structure 105 in file .gra /

AB The influence of 27 possible effectors, mostly bispyridinium salts, on the dealkylation (aging) of soman-inhibited acetylcholinesterase was examined at pH 7.6 and 25°. In the absence of effectors, the rate constant of the aging process was 4.0 + 10<sup>-2</sup> min<sup>-1</sup>. At 2 mM, the strongest inhibitor reduced the rate to 0.8 + 10<sup>-2</sup> min<sup>-1</sup>, whereas it was raised to 8.2 + 10<sup>-2</sup> min<sup>-1</sup> by the most potent accelerator.

L5 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN  
ACCESSION NUMBER: 1970:402338 CAPLUS  
DOCUMENT NUMBER: 73:2338  
TITLE: Relation between chemical structure and cholinesterase reactivating effect in a number of new asymmetric bis-quaternary pyridinium salts. I. Derivatives of 4-hydroxyiminomethylpyridine  
AUTHOR(S): Dirks, E.; Scherer, A.; Schmidt, Max; Zimmer, Gerhard  
CORPORATE SOURCE: Battelle-Inst. e.V., Frankfurt/M., Fed. Rep. Ger.  
SOURCE: Arzneimittelforschung (1970), 20(1), 55-62

CODEN: ARZNAD; ISSN: 0004-4172

DOCUMENT TYPE: Journal

LANGUAGE: German

IT 27844-72-0 31984-53-9

RL: BIOL (Biological study)  
(cholinesterase reactivation by)

RN 27844-72-0 CAPLUS

CN Pyridinium, 3-(dimethylamino)-1-[[[4-[(hydroxyimino)methyl]pyridinio]methoxy]methyl]-, dichloride (9CI) (CA INDEX NAME)

/ Structure 106 in file .gra /

RN 31984-53-9 CAPLUS

CN Pyridinium, 3-amino-4'-formyl-1,1'-(oxydimethylene)di-, dichloride, oxime  
(8CI) (CA INDEX NAME)

/ Structure 107 in file .gra /

AB Two series of asymmetric bis(pyridinium) salts, characterized by a methylene or O link joining the N atoms of the pyridine nuclei and having a p-aldoxime substituent on 1 of the pyridine nuclei were **synthesized**, including 1-[3-(3-dimethylamino-1-pyridinyl)propyl]-pyridine-4-aldoxime dibromide, 1-[3-(3-fluoro-1-pyridinyl)-2-oxapropyl]pyridine-4-aldoxime dichloride, 1-[3-(4-methoxy-1-pyridinyl)propyl]pyridine-4-aldoxime dibromide, and 1-[3-(4-tert-butylpyridinyl)-2-oxapropyl]pyridine-4-aldoxime dichloride. The ability of these compds. to reactivate acetylcholinesterase, previously inhibited by diisopropylfluorophosphate, as well as their inhibitory effect on untreated enzyme, depended on the radical added to the pyridine nuclei and on the nature of the bridge member. The size of the radical and its ability to dissociate into ions appear to be the essential factors, the electronic and phys. properties characterized by the Hammett  $\sigma$ -consts. and the Rf values being less important. The aldoxime radical had little effect on the activity of these compds., since it could be replaced by other radicals without affecting the results substantially. No significant relations between the increase in the hydrolysis rate of diisopropylfluorophosphate in the presence of bis(pyridinium) salts and their reactivating effect, or between the acute toxicity of the salts and their inhibitory effects on acetylcholine-esterase, were observed

L5 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1970:111249 CAPLUS

DOCUMENT NUMBER: 72:111249

TITLE: Relation between chemical structure and cholinesterase reactivating effect in new asymmetric pyridinium salts. II. Derivatives of 2-hydroxyiminomethylpyridine

AUTHOR(S): Dirks, E.; Scherer, A.; Schmidt, Max; Zimmer, Gerhard

CORPORATE SOURCE: Battelle-Inst. e. V., Frankfurt/M., Fed. Rep. Ger.

SOURCE: Arzneimittel-Forschung (1970), 20(2), 197-200

CODEN: ARZNAD; ISSN: 0004-4172

DOCUMENT TYPE: Journal

LANGUAGE: German

IT 27183-61-5P 27183-62-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 27183-61-5 CAPLUS

CN Pyridinium, 3'-amino-2-formyl-1,1'-(oxydimethylene)di-, dichloride, oxime

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(8CI) (CA INDEX NAME)

/ Structure 108 in file .gra /

RN 27183-62-6 CAPLUS

CN Pyridinium, 1-[[[3-(dimethylamino)pyridinio]methoxy]methyl]-2-  
[(hydroxyimino)methyl]-, dichloride (9CI) (CA INDEX NAME)

/ Structure 109 in file .gra /

GI For diagram(s), see printed CA Issue.

AB I (Q = CH<sub>2</sub> or O; R = m- or p-NO<sub>2</sub>, MeSO<sub>2</sub>, F, Cl, Br, I, SMe, NH<sub>2</sub>, NMe<sub>2</sub>,  
tert-Bu, MeO; CH:NOH, CO<sub>2</sub>H, or CHN+Me<sub>3</sub>; X = Cl or Br) were **prepd**  
. by authors' (1970) methods. I with R in the m-position did not  
reactivate acetylcholinesterase (EC. 3.1.1.7) inhibited with diisopropyl  
fluorophosphate. I (R = p-tert-Bu) showed significant reactivating  
activity at 1.05 e 10<sup>-2</sup> M. The reactivating activity of all I was lower  
than that of the corresponding p-aldoximes. I with large or polar  
R-substituents showed the lowest inhibiting activity on  
acetylcholinesterase. I (Q = O, R = m-substituent) showed the greatest  
inhibiting activity.

=> log y

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ENTRY	SESSION
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